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Turbulent Spray Combustion Modeling for Rocket Engine Applications

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Abstract

The paper concerns the modeling of turbulent liquid oxygen/hydrogen spray combustion for elevated subcritical pressure and cryogenic inlet temperature conditions. Various approaches are outlined and discussed that concern current and future models for turbulent two-phase flows as well as models to include detailed chemical reactions. The presence of the liquid phase complicates the situation since the turbulence and the chemical reactions not only interact with each other but also with the spray processes. After the presentation and discussion of general approaches, the combustion in a single injector combustion chamber is modeled where experimental data are available for gas phase temperature and both droplet size and velocities. The model uses an Eulerian-Lagrangian formulation for the gas and the liquid phase, respectively. Detailed models for droplet heating and vaporization in a convective flow field are employed, and detailed gas phase reactions are accounted for through use of a flamelet model for turbulent spray combustion. The results show a very good agreement between experimental and computational spray characteristics. The computed gas phase temperature lies above the experimental values which is associated with CARS single shot measurements and incomplete data for the initial conditions of the combustion process.

1 Introduction

An improved understanding of the physical and chemical processes occurring in liquid rocket engines is required to ensure the stability, reliability, and efficiency of their performance. The gaseous hydrogen and the liquid oxygen (LOX) are injected at cryogenic inlet temperatures, and the turbulent combustion occurs in both the sub- and supercritical domain. Therefore, the models for the processes in systems such as the Ariane V or the Space Shuttle main engine are very complex. The paper concerns principal approaches to the modeling of these processes and discusses the state of the art as well as potential approaches in future.

Finally, the combustion process in a single injection combustion chamber is investigated for elevated pressure and cryogenic inlet temperatures. Experimental data are available for an elevated pressure situation of 5 bar, and the experimental data are published by Sender *et al.* [1]. The combustion in liquid rocket propulsion typically occurs in the flamelet regime of turbulent combustion [2] which enables the use of the flamelet model for turbulent spray diffusion flames [3, 4]. Structures of laminar hydrogen/oxygen flames are precalculated at 5 bar and for cryogenic inlet temperature of 100 K for hydrogen [5, 6]. They are incorporated into the turbulent spray combustion model which allows the computation of all chemical species

that are included in the detailed chemical reaction mechanism for the hydrogen/oxygen system that includes 8 reactive species and 38 chemical reactions [7].

2 Turbulence Modeling of Two-Phase Flows

Two-phase flows are characterized by the separation of the turbulent flow field and the strong interaction between the spray and the gas through processes such as turbulent mixing, droplet heating, vaporization, and motion as well as coupling with possible occurrence of chemical reactions. In practical systems, most often the turbulent gas flow is modeled using a $k - \epsilon$ turbulence model where additional terms are added to account for the interaction with the liquid. This formulation is done within an Eulerian-Lagrangian formulation of governing equations for a dilute spray within either a discrete droplet or a continuous droplet model, c.f. Faeth [8]. An example of the mathematical equations within a discrete droplet model is given through [3]

$$L(\tilde{\Phi}) \equiv \frac{\partial(\bar{\rho}\tilde{u}\tilde{\Phi})}{\partial x} + \frac{1}{r} \frac{\partial(\bar{\rho}\tilde{v}\tilde{\Phi})}{\partial r} - \frac{\partial}{\partial x} \left(\frac{\mu_{\text{eff}}}{\sigma_{\Phi}} \frac{\partial \tilde{\Phi}}{\partial x} \right) - \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\mu_{\text{eff}}}{\sigma_{\Phi}} \frac{\partial \tilde{\Phi}}{\partial r} \right) = L_{\text{gas},\tilde{\Phi}} + L_{\text{spray},\tilde{\Phi}} \quad (1)$$

where the source terms are given in Tab. 1. Here a two dimensional axisymmetric configuration is considered where x and r denote the axial and radial directions, respectively. Favre averaged values are used.

| Variable | $\tilde{\Phi}$ | $L_{\text{gas},\tilde{\Phi}}$ | $L_{\text{spray},\tilde{\Phi}}$ |
|---|--------------------|--|---|
| Mass | 1 | 0 | $\sum_{k=1}^{N_p} (n\dot{m})_{p,k} \equiv \bar{L}_v$ |
| Momentum in Axial Direction | \tilde{u} | $-\frac{\partial \bar{p}}{\partial x} - \frac{2}{3} \frac{\partial}{\partial x} \left[\mu_{\text{eff}} \left(\frac{\partial \tilde{u}}{\partial x} + \frac{1}{r} \frac{\partial(r\tilde{r})}{\partial r} \right) \right] + \bar{\rho}g$ | $\sum_{k=1}^{N_p} (n\dot{m}u)_{p,k}$ |
| Momentum in Radial Direction | \tilde{v} | $-\frac{\partial \bar{p}}{\partial r} - \frac{2}{3} \frac{\partial}{\partial r} \left[\mu_{\text{eff}} \left(\frac{\partial \tilde{u}}{\partial x} + \frac{1}{r} \frac{\partial(r\tilde{r})}{\partial r} \right) \right] - 2 \frac{\mu_{\text{eff}} \tilde{r}}{r^2}$ | $\sum_{k=1}^{N_p} (n\dot{m}v)_{p,k}$ |
| Energy | \tilde{h} | 0 | $\sum_{k=1}^{N_p} (n\dot{m}h)_{p,k}$ |
| Mixture Fraction | ξ | 0 | \bar{L}_v |
| Variance of the Mixture Fraction | $\tilde{\xi'^2}$ | $2\Gamma_{\xi'^2} \text{div}^2 \tilde{\xi} - 2\bar{\rho}\tilde{\epsilon} / \tilde{k} \tilde{\xi'^2}$ | $\bar{L}_v \tilde{\xi'^2} (1 - 2\tilde{\xi}) / \tilde{\xi}$ |
| Turbulent Kinetic Energy | \tilde{k} | $G_k - \bar{\rho}\tilde{\epsilon}$ | $\sum_{k=1}^{N_p} \tilde{u}''(n\dot{m}\tilde{v})_{p,k}$ |
| Dissipation Rate of the Turbulent Kinetic Energy | $\tilde{\epsilon}$ | $(C_1 G_k - C_2 \bar{\rho}\tilde{\epsilon})\tilde{\epsilon} / k$ $G_k = -\overline{\rho u'' \otimes u''} : \text{grad} \tilde{u}$ | $\epsilon / k L_{\text{spray},\tilde{k}}$ |

Table 1: Source terms for Eq. 1 [3].

| | ϕ | $j_{\phi,k}$ | $T_{\phi,k}$ | S_{ϕ} | L_{ϕ} | |
|------------------|--------------|--|--------------|---|---|----------------------|
| Continuity | 1 | 0 | 0 | 0 | L_v | |
| Momentum | v_i | 0 | τ_{ik} | $-\frac{\partial p}{\partial x_i} + \rho g_i$ | $L_{m,i}$ | $i = 1 \dots 3$ |
| Enthalpy | h | $-\frac{\lambda}{c_p} \frac{\partial h}{\partial x_k}$ | 0 | 0 | L_e | |
| Mass Fractions | Y_{α} | $-\rho D \frac{\partial Y_{\alpha}}{\partial x_k}$ | 0 | ω_{α} | $L_{v,\alpha}$ | $\alpha = 1 \dots N$ |
| Element Mass Fr. | Z_j | $-\rho D \frac{\partial Z_j}{\partial x_k}$ | 0 | 0 | $\sum_{\alpha=1}^N \mu_{j,\alpha} L_{v,\alpha}$ | $j = 1 \dots M$ |

Table 2: Source terms for Eq. 2 [12].

Even though this model is used in most technical simulations, it has major drawbacks such as the well known problem of the $k - \epsilon$ model in strongly recirculating flows and its failure of modeling anisotropic turbulence which is common to all models using the turbulence energy k . Moreover, the model is based on a gradient diffusion assumption which is not appropriate to predict the effect of counter gradient diffusion which has been observed in turbulent gas flows.

More advanced models that are under investigation in gas phase flows are currently extended to two-phase flows. These are the LES – Large Eddy Simulation, the Reynolds stress models, and DNS – Direct Numerical Simulation. There is a special presentation [9] at the present meeting that deals with LES, and therefore this approach is not discussed within the frame of this presentation. The method of DNS is currently applied to small problems – small in the sense of physical dimensions of the system investigated [10] since the entire range of length scales needs to be resolved which restricts the dimension of the problem. However, the method is very interesting when well defined submodels are to be investigated.

The Reynolds stress models are typically used when non-isotropic turbulence occurs and if counter gradient diffusion is present. The model does not use the k equation but transport equations for the Reynolds stress terms $\overline{u_i'' u_j''}$. Additional terms appear that describe the coupling between the velocity fluctuations and the spray source terms that stem from droplet heating, vaporization, and motion. The Reynolds stress equations yield

$$\begin{aligned}
 \frac{\partial(\bar{\rho}\psi''\phi'')}{\partial t} + \frac{\partial(\bar{\rho}\tilde{v}_k\psi''\phi'')}{\partial x_k} = & \underbrace{-\bar{\rho}v_k''\psi''\frac{\partial\tilde{\phi}}{\partial x_k}}_{\text{I}} - \underbrace{\bar{\rho}v_k''\phi''\frac{\partial\tilde{\psi}}{\partial x_k}}_{\text{II}} - \underbrace{\frac{\partial(\bar{\rho}v_k''\psi''\phi'')}{\partial x_k}}_{\text{II}} \\
 & \underbrace{-\phi''\frac{\partial}{\partial x_k}(j_{\psi,k} + T_{\psi,k}) - \psi''\frac{\partial}{\partial x_k}(j_{\phi,k} + T_{\phi,k})}_{\text{III}} + \underbrace{\overline{\phi''S_{\psi}} + \overline{\psi''S_{\phi}}}_{\text{IV}} \\
 & \underbrace{-L_v(\phi''\psi'' + \tilde{\phi}\psi'' + \tilde{\psi}\phi'') + \overline{\phi''L_{\psi}} + \overline{\psi''L_{\phi}}}_{\text{V}},
 \end{aligned} \tag{2}$$

and the source terms are given in Tab. 2:

For completeness and further use in the next section, the element mass fraction, Z_j , is also shown in the Tab. 2. The terms I to IV in Eq. 2 may be closed using the standard models for pure gas phase equations whereas the terms V describe the interaction between the spray and the variable under consideration. These terms may be formulated according to the derivations in Ref. [3, 4], and they are currently under investigation.

Another approach is that of Burlaka and Borghi [11] that describes the spray surface, \sum_i , with a transport equation

$$\frac{d}{dt} \left(\overline{\sum_i} \right) + \frac{d}{dx_k} \left(u_k \overline{\sum_i} \right) = \text{diffusion} + \text{production} + \text{destruction}. \quad (3)$$

The destruction term includes the vaporization process. This model is motivated by the surface transport equation in turbulent premixed combustion, and the description of the vaporization process is still under development.

3 Models for Chemical Reactions in Turbulent Reactive Two-Phase Flows

The chemical reactions in a convective flow field may be described mathematically through the conservation equation of the mass fractions, Y_i , of chemical species i :

$$\frac{\partial(\rho Y_i)}{\partial t} = - \frac{\partial(\rho_i u_{ik})}{\partial x_k} + M_i \dot{w}_i + \delta_{iL} L_v, \quad (4)$$

where \dot{w}_i is the molar chemical reaction rate and L_v is the source term due to liquid vaporization. δ_{iL} is the Dirac-Delta function where L denotes the species in liquid phase. The system of chemical reactions is written as

$$\sum_{i=1}^M \nu'_{ij} \mathcal{M}_i \rightleftharpoons \sum_{i=1}^M \nu''_{ij} \mathcal{M}_i, \quad j = 1, \dots, N, \quad (5)$$

and the consumption/production rate of a chemical species yields

$$\dot{w}_i = \sum_{j=1}^N (\nu''_{ij} - \nu'_{ij}) w_j, \quad i = 1, \dots, M, \quad (6)$$

where w_j is the reaction rate of a reaction step, j , using the modified Arrhenius expression for the reaction constant

$$w_j = A_j T^{b_j} e^{E_j/(RT)} \prod_{i=1}^M [Y_i p \bar{M}_i / (RT M_i)], \quad j = 1, \dots, N \quad (7)$$

for N chemical reaction steps.

If the chemical reactions are to be modeled using a mixture fraction, the source term due to chemical reactions disappears. The mixture fraction may be based on the elements, i , present in the system:

$$\xi(i) = \sum_{j=1}^M \mu_{ij} (Y_j - Y_{j\infty}) / \sum_{j=1}^M \mu_{ij} (Y_{j-\infty} - Y_{j\infty}), \quad (8)$$

where $i = \text{N, O, H}$, and μ_{ij} is the mass of element i in molecule j . The mixture fraction may also be based on enthalpy [13]

$$\xi(h) = \frac{\sum_{i=1}^M (Y_i h_i - Y_{i\infty} h_{i\infty})}{\sum_{j=1}^M (Y_{j-\infty} h_{j-\infty} - Y_{j\infty} h_{j\infty})}. \quad (9)$$

If the Lewis numbers of all species were unity, then there is no difference in the above definitions. However, for the hydrogen/oxygen system, this is not true, and some of the definitions show unreasonable values [13]. In the remainder of the paper, the mixture fractions is based on the element H which is the best choice in terms of monotonicity with physical space for the hydrogen/oxygen system.

Taking these definitions for the instantaneous values of the chemical reaction rate, there are various approaches to close the problem in turbulent reactive flows. The directest approach is the direct closure of the source term of chemical reactions through use of a joint probability density function (PDF), P , leading to the following averaged chemical reaction rate:

$$\overline{M_i \dot{w}_i} = M_i \int_0^1 \dots \int_0^1 \int_0^\infty \int_0^\infty \dot{w}_i P(Y_1, \dots, Y_N, p, T) dT dp dY_1 \dots dY_N. \quad (10)$$

Since the joint PDF is not known, most often it is factorized and beta functions are used to describe to single PDFs

$$\tilde{P}(\tilde{\Phi}) = \frac{\Gamma(\alpha + \beta)}{\Gamma(\alpha)\Gamma(\beta)} \tilde{\Phi}^{\alpha-1} (1 - \tilde{\Phi})^{\beta-1}. \quad (11)$$

The α and β are linear functions of the variance of the variable Φ under consideration, and they are obtained through solution of their transport equations, c.f. Eq. 2.

Most often this approximation is not too bad in gas phase combustion. However, it appears [10] that the beta-function is a poor approximation in regimes where the vaporization occurs. Therefore, new approaches need to be developed.

A promising approach seems to be the formulation through a PDF transport equation. This model has been developed by Pope [14] and Dopazo [15] for gas phase combustion. The PDF is modeled through a transport equation, and the chemical source terms may be used without the averaging procedure described above. The formulation of the PDF transport equation for the PDF of the mixture fraction, P_ξ , yields for turbulent two-phase flows

$$\begin{aligned} \frac{\partial(\rho P_\xi)}{\partial t} + \frac{\partial}{\partial x_i} (\rho U_i P_\xi) + \frac{\partial}{\partial x_i} (\langle \rho u'_i | \xi = \phi \rangle P_\xi) = \\ \frac{\partial^2}{\partial \phi^2} \left[\rho D \left\langle \frac{\partial \xi}{\partial x_i} \frac{\partial \xi}{\partial x_i} \right| \xi = \phi \right] P_\xi + \frac{\partial}{\partial x_i} \left(\rho D \frac{\partial P_\xi}{\partial x_i} \right) - \frac{\partial}{\partial \phi} (L_v P_\xi) \end{aligned} \quad (12)$$

where the third term on the LHS is usually modeled using

$$\langle \rho u'_i | \xi = \phi \rangle P_\xi = -\frac{\eta}{\sigma_\xi} \frac{\partial P_\xi}{\partial x_i}. \quad (13)$$

This approach has not yet been investigated for turbulent two-phase flows to the author's knowledge, but it appears promising. The diffusion term needs to modeled using particle mixing models, and it is unclear if they can be used for two-phase flows without modification.

The major advantage of this approach is that the PDF transport equation needs no information on fluctuations of the droplet vaporization, and it enables the evaluation of a PDF that may possibly be approximated through an extension of well known standard PDFs. For reactive flows, the approach is beneficial because it does not require averaged chemical reaction terms – the instantaneous values are sufficient.

The chemistry itself may be included through use of detailed reaction schemes [7], reduced reaction mechanisms [16], or tabulated systems such as the ILDM approach [17]. There is a number of reduced chemical reaction schemes for the hydrogen/oxygen system, and they range from 4-step to 2-step schemes [16]. The chemical reactions in high pressure systems typically occur with small time scales so that the use of a lower number of reaction steps is more justified as pressure increases, and for very high pressure even a one-step mechanism performs well.

Another type of model to include detailed chemical reactions is the flamelet model for turbulent combustion [18, 19, 20] which has been extended for turbulent spray diffusion flames [3, 4]. The model considers the turbulent flame to consist of an ensemble of laminar flamelets that are stretched through the turbulence of the flow field, c.f. Fig. 1.

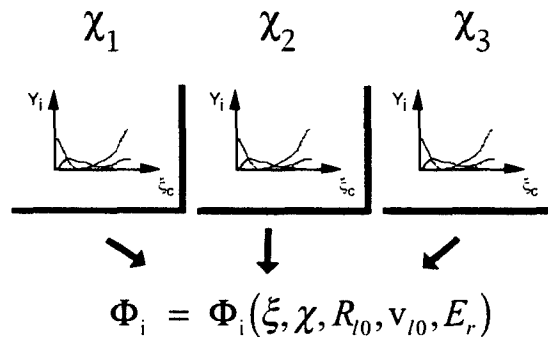


Figure 1: Schematic of the flamelet model for turbulent spray combustion.

The laminar flamelet depends on the mixture fraction, ξ , the scalar dissipation rate, χ , the initial droplet size and velocity, R_{l0} and v_{l0} , resp., and the equivalence ratio, E_r . The Favre averaged values of a variable, Φ , then yields [4]

$$\tilde{\Phi} = \int_0^\infty \int_0^\infty \int_0^\infty \int_0^\infty \int_0^1 \Phi(\xi, \chi, R_{l0}, v_{l0}, E_r) \tilde{P}(\xi, \chi, R_{l0}, v_{l0}, E_r) d\xi d\chi dR_{l0} dv_{l0} dE_r. \quad (14)$$

The joint probability density function is factorized, and the one-dimensional PDFs need to be determined [4]. Currently, there are libraries available for the liquid oxygen/hydrogen system [6] and for the methanol/air [21] and ethanol/air [22] systems.

In the following section, the flamelet model for turbulent spray diffusion flames is used together with the model described through the equations given in Tab. 1 to simulate the combustion process in the micro combustion chamber M3 of the DLR in Lampoldshausen [23].

4 Simulation of the Combustion Process in the Micro Combustion Chamber M3

4.1 Model

A dilute LOX spray is considered that is injected into a turbulent gaseous hydrogen stream where the inlet temperatures are cryogenic. The system pressure is 5 bar. The model includes an Eulerian description of the gas phase and Lagrangian equations for the dilute spray. The $k - \epsilon$ turbulence model is employed where additional terms account for the spray interaction [3], c.f. Tab. 1. The chemical reactions are described through a flamelet model for turbulent spray diffusion flames [3, 4] outlined in the previous section. The conservation equations for the mixture fraction and its variance also account for mass gain through vaporization of the liquid [3].

Convective heating and vaporization is described through a model developed by Abramzon and Sirignano [24]. The equation for droplet motion accounts for turbulence effects through a Gaussian distribution for turbulent fluctuations [25]. The spray distribution is described through the discrete droplet model [23].

For the computation of the gas phase characteristics in the cryogenic temperature regime, data from JSME tables [26] for pressures up to 200 bar and temperatures between 80 and 300 K are used. Moreover, the pressure (and temperature) dependence of the vaporization rate and of the binary equilibrium composition at the liquid/gas interface [27] is included. For the pressure considered here, the real gas effects in the gas phase are negligible [28].

4.2 Results and Discussion

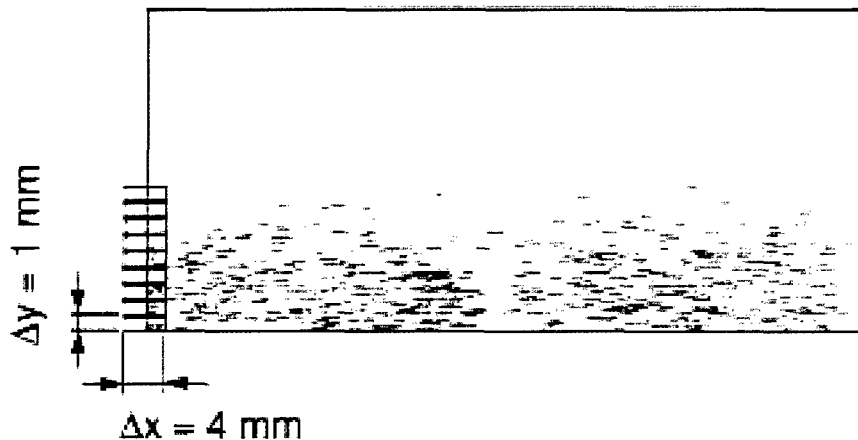


Figure 2: Measured droplet velocities in the range between 72 and 140 mm from their injector [1].

The experimental data [1, 23] include gas temperature as well as droplet velocities and size. Figure 2 displays the droplet velocities obtained from experiment using PIV. The area displayed ranges from 72 mm to 140 mm of the combustion chamber which is the second half of the entire single-injector micro combustion chamber M3 of the DLR in Lampoldshausen,

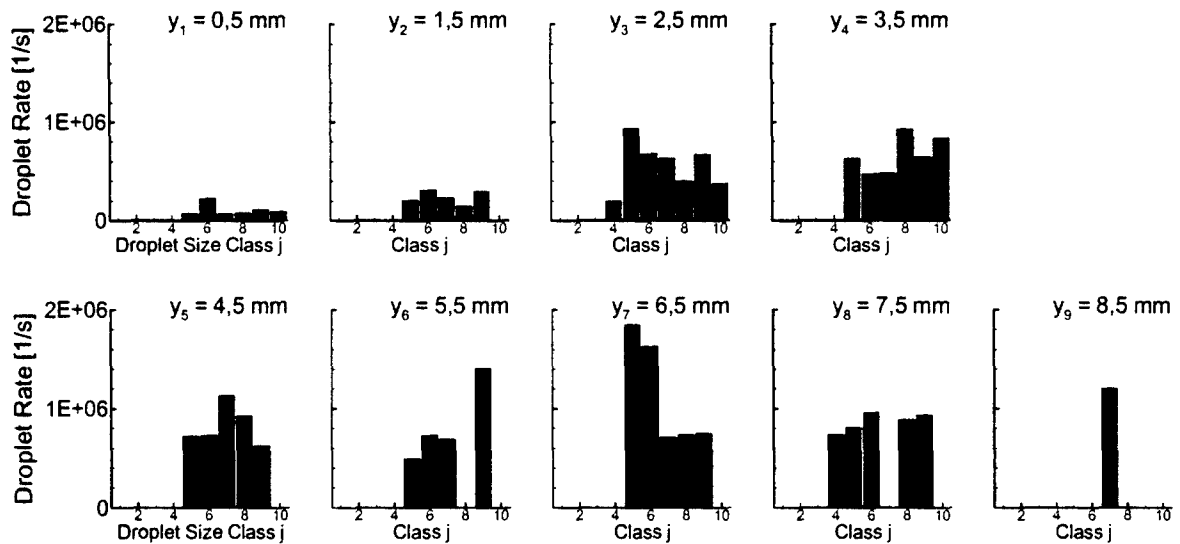


Figure 3: Initial droplet rate and distribution for 9 different size classes evaluated from experimental data [1] at $x = 72$ mm from the injector [23].

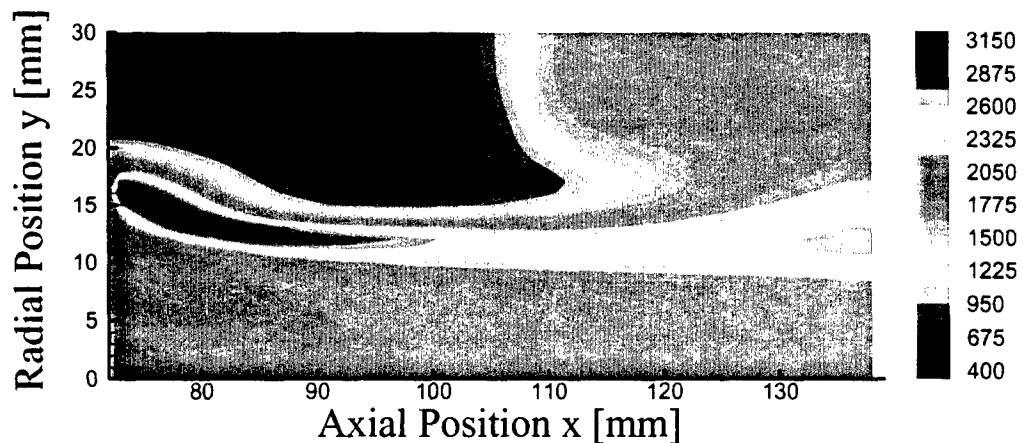


Figure 4: Contour plot of the gas temperature [23].

Germany. In the first part of the combustor, the spray is rather thick, and the model is not suitable. The experimental data are used to produce initial profiles for the simulation as well as for comparison further downstream in the combustion chamber.

Figure 3 shows the generated initial droplet rate at the axial position 72 mm. The depth of field in the experiment is 0.5 mm which has been used to calculate the droplet rate. The experiment typically does not comprise more than about 15 % of the entire liquid. Sometimes in the literature, this value is extrapolated to 100% and there are several methods to do so. However, we preferred to stick to the experimental data that we received since there is no reliable information about how much of the liquid flux exactly needs to be compensated for which causes a second ambiguity in the procedure.

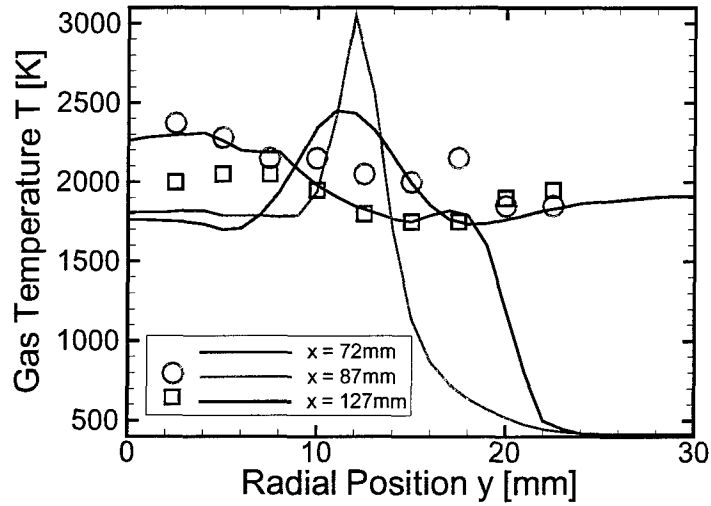


Figure 5: Radial profiles of the gas temperature for three different axial positions: Symbols present experimental data and lines show computational results [23].

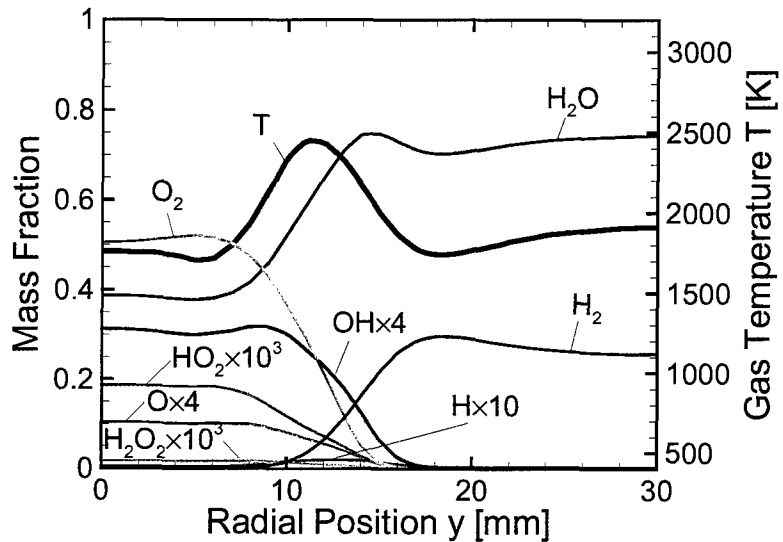


Figure 6: Radial profiles of the gas temperature and species mass fractions at $x = 127$ mm [23].

Also, there are no gas temperature measurements exactly at $x = 72$ mm, and the inlet conditions for the gas temperature have been obtained from interpolated experimental data at two surrounding axial positions. Moreover, the experimental data have been extrapolated into the outer regions where no experimental data are available.

There is no information on other gas phase characteristics such as species concentrations from the experiment. The initial gas velocity is taken from the experimental velocity of the smallest droplets, and the species profiles are estimated from the experimental gas temperature. The turbulence quantities k and ϵ are computed from the gas phase velocity.

Figure 4 shows the computed overall structure of the spray flame in terms of the computed

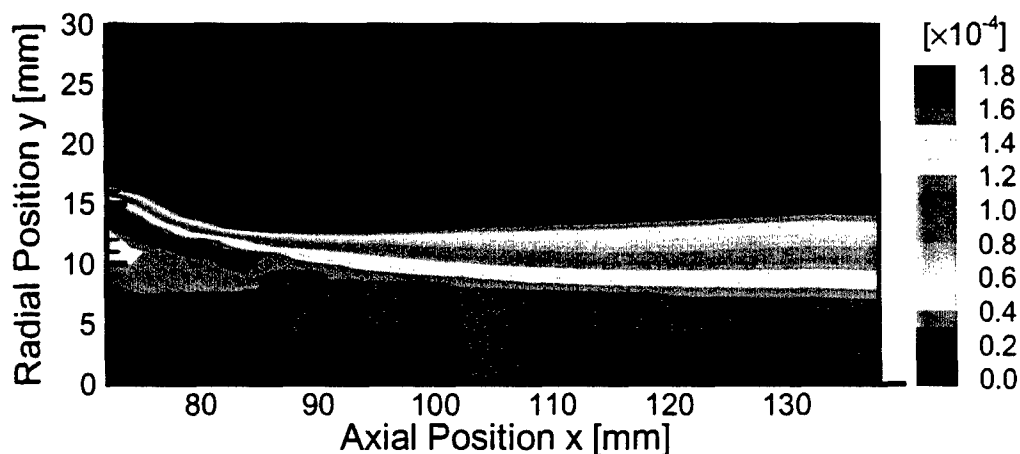


Figure 7: Contour plot of the mass fraction of HO_2 [23].

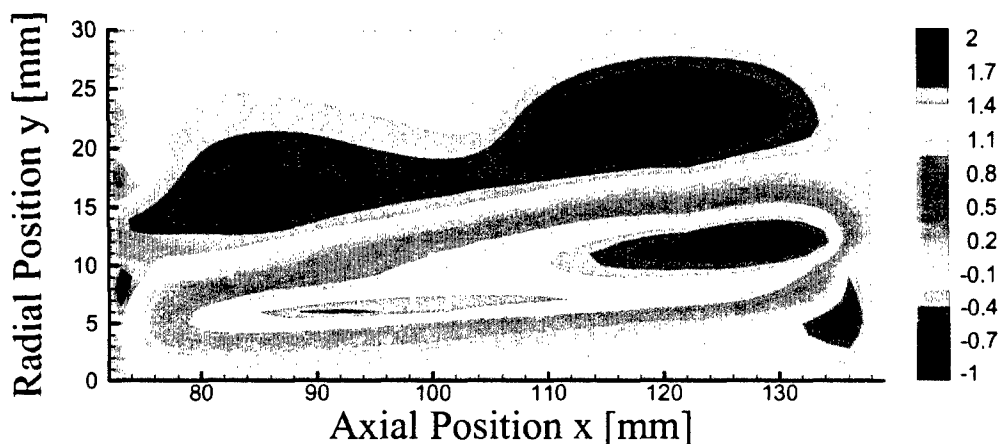


Figure 8: Contour plot of the radial gas velocity [23].

gas phase temperature. The main chemical reaction zone is located at the boundary of the spray jet where vaporized oxidizer meets the surrounding hydrogen gas stream. The maximum flame temperature is about 3000 K which is typical for these high-pressure flames.

A more detailed investigation of flame temperature is shown in Fig. 5 where the calculated and experimental radial profiles of the gas temperature are shown for three different axial positions. Symbols show experimental data and lines are computational results.

Figure 5 shows that the gas temperature in the main reaction zone is overpredicted by the computations. This may be attributed to both experimental and computational uncertainties. First the experiments employed CARS single shot measurements, and the averaging procedure of these values typically leads to an underprediction of the measured gas temperatures. Moreover, the initial gas phase profiles needed for the computations is estimated from the gas temperature profile, and this procedure is somewhat arbitrary. Another reason is to be found in the incomplete liquid phase data as discussed earlier. The computations use the uncorrected data from measurements so that the vaporization of the

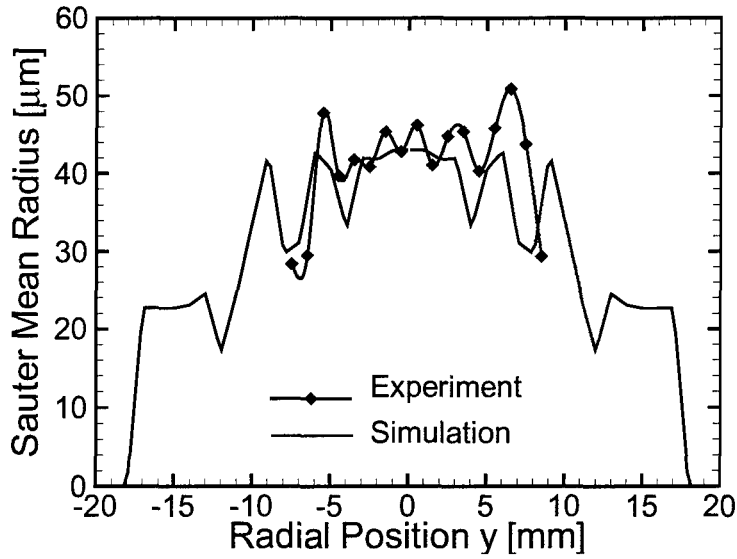


Figure 9: Experimental and computational results of the Sauter mean radius at $x = 104$ mm [23].

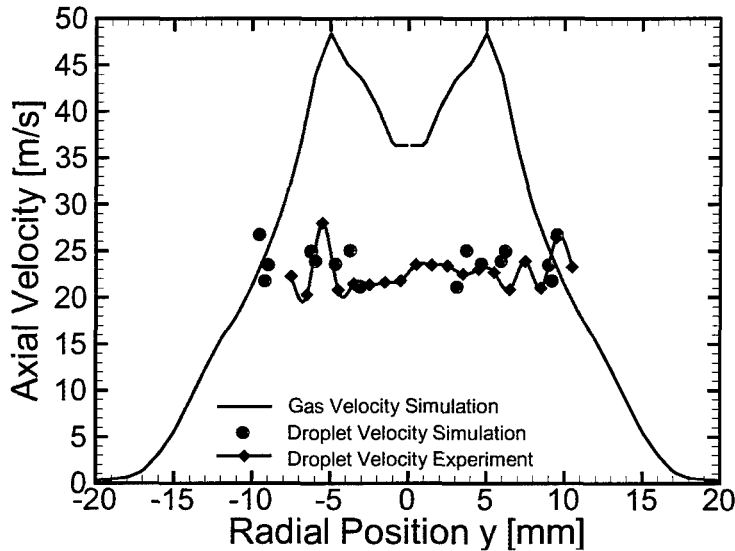


Figure 10: Experimental and computational results of the droplet velocities as well as calculated gas velocities at $x = 104$ mm [23].

neglected liquid would reduce the gas phase temperature. Therefore, the discrepancies of computed and measured temperature profiles in the gas phase is reasonable.

The flamelet model is suitable to predict all species profiles that are considered in the laminar flamelet library. Figure 6 shows radical profiles at $x = 127$ mm. The HO_2 and H_2O_2 are present in the colder flame region (due to their stability) near the axis of symmetry where molecular oxygen in the gas phase is present. The location of the H_2O peak is shifted to the fuel side which is typical for gas phase combustion. Figure 7 shows the contour plot of the HO_2 mass fraction, and the differences compared to the gas temperature contour plot are obvious. The HO_2 prevails into the colder regions of the combustion chamber favorably in regions where gaseous O_2 is present.

The gas phase velocities show that there is a region where recirculation occurs. This may be seen in Fig. 8 where the radial gas phase velocity is displayed. This finding is in agreement with experiment [1]. It is well known that the $k - \epsilon$ turbulence model that is used here is not the best choice if recirculation is present, and a future study will include a Reynolds stress model for turbulent spray flames.

Figures 9 and 10 show a comparison of liquid phase characteristics. Figure 9 displays the radial profile of the Sauter mean radius at $x = 104$ mm. Symbols mark experimental results, and the agreement between experiment and computation is excellent. The same is true for the profiles of axial velocities at the same axial position plotted in Fig. 10. Thus it is shown that the present model is suitable to correctly predict the liquid phase properties.

5 Summary and Future Research

The combustion process in the micro combustion chamber M3 has been studied by means of numerical computations. The Eulerian/Lagrangian model is suitable to predict the processes in the dilute spray regime of the combustion chamber. In particular, the prediction of the spray distribution and evolution is very good.

Calculated gas phase temperatures are higher than the experimental values which is explained by various reasons. First, the experimental data are probably underpredicted which is typical for CARS single shot measurements. Moreover, only a small portion of the total liquid flux was captured by the experimental techniques so that the energy consumed by droplet vaporization is underpredicted leading to too high values of gas temperature in the computation. Furthermore, there is no information of gas phase species profiles from experiment leading to uncertainties in evaluating the initial conditions for the computations.

Future studies should include the dense spray regime, and an extension of the present model into that region will be developed.

Moreover, the Reynolds stress model for turbulent spray flames will be employed to account for an improved simulation of the recirculation zone. Here the coupling terms of velocities and vaporization fluctuations need to be modeled.

In future, the pressure will also be increased into the high-pressure domain.

6 Acknowledgments

Financial support of the Deutsche Forschungsgemeinschaft through SFB 359 is gratefully acknowledged.

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